Research Article

Topological Descriptors on Some Families of Graphs

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In view of the successful applications of graph theory, relationships between the biological activity and chemical structure have been developed. One of the popular topics in graph theory is problems relating to topological indices. Degree-based topological indices, distance-based topological indices, and counting-related topological indices are various types of topological indices. Physiochemical properties such as boiling point and stability of chemical compounds are correlated by these topological indices. A topological index of a graph is a numerical quantity obtained from the graph mathematically. A cactus graph is a connected graph in which no edge lies in more than one cycle. In this study, we have derived certain degree-based topological indices for some families of graphs consisting of graph obtained by the rooted product of paths and cycles and two types of cactus graph (paracactus and orthocactus) with the help of the generalized Zagreb index.

1. Introduction

Let G be a graph, $V(G)$ be vertices of G , and $E(G)$ be the edge of G ; then, the total number of vertices in G is called the order of G , and the total number of edges in G is called the size of G ; any edge having the same starting and ending vertex is called a loop. In a graph, if two or more edges have the same starting and ending vertex, then we call this multiple edge. A graph which does not contain a loop or multiple edge is called a simple graph, and a graph which contains a loop or multiple edge is called a multigraph. A graph G is a planar graph if we draw it into the plane without any edge intersection. If it is not possible, then we call it a nonplanar graph. In a graph G , from one vertex to another vertex, we give orientation or directions to each edge; then, this graph is called a directed graph; if we start moving from one vertex and, after travelling different edges, we reach back that vertex, then it forms a cycle. If a graph has no cycle, then we call it a tree. Spanning tree is a subgraph which has the

same vertex as the original graph. In this paper, we use undirected graphs. Graph theory was successfully employed through the translation of chemical structures into characteristic numerical descriptors by resorting to graph invariants. A graph invariant is any function on a graph that does not depend on labeling of its vertices. Such quantities are also called topological indices. Hundreds of different invariants have been employed to date in QSAR/QSPR studies. Among more useful of them appear two that are known under various name. Topological indices are numerical parameters of a graph which are invariant under graph isomorphism. Interest in the field of computational chemistry in topological indices has been on the rise for a considerable length of time. A graph can be recognized by a numerical number, a polynomial, an arrangement of numbers, and either a network or a matrix which represents the whole graph. A topological index is a numerical amount related to a graph, which describes the geography of the graph and is invariant under diagram automorphism [1–7].

There are some significant classes of topological indices, for example, distance-based topological indices, degree-based topological indices, and eccentricity-based and counting-related polynomials and indices of the graph. Among these classes, degree-based topological indices have overwhelming significance and perform a pivotal role in the preparation of graph hypothesis, especially in science. If it is made more precise, a topological list $\text{Top}(G)$ of a graph is a number with the property that, for each graph H isomorphic to G , $\text{Top}(H) = \text{Top}(G)$. The concept of topological indices came from Wiener when he was studying the boiling point of a member of the alkene family, called paraffins. He named this topological index the path number. When research in chemical graph theory progressed, the name Wiener index was given to the path number. Owing to its interesting theoretical properties and wide range of applications, the Wiener index is the most investigated molecular topological index in chemical graph theory [8, 9]. The first and the second Zagreb indices were introduced by Gutman and Trinajestić [10]. H. Wiener gave the concept of the topological index, namely, as the Wiener index [11] and is defined as

$$W(G) = \frac{1}{2} \sum_{pq \in E(G)} d(p, q). \quad (1)$$

The chemist Randić introduced a topological index under the name branching index:

$$R_\alpha(G) = \sum_{pq \in E(G)} [d(p)d(q)]^\alpha. \quad (2)$$

Vukicević and Furtula et al. introduced one of the well-known connectivity topological indices, namely, atom-bond connectivity (ABC) index [12], defined as

$$\text{ABC}(G) = \sum_{pq \in E(G)} \sqrt{\frac{d(p)d(q) - 2}{d(p)d(q)}}. \quad (3)$$

Nikolić et al. [13] introduced Zagreb indices defined as

$$\begin{aligned} M_1(G) &= \sum_{p \in V(G)} \delta(p)^2, \\ M_2(G) &= \sum_{p, q \in V(G)} \delta(p)\delta(q). \end{aligned} \quad (4)$$

Vukićević and Furtula [12] introduced another well-known connectivity topological descriptor, namely, geometric-arithmetic (GA) index:

$$\text{GA}(G) = \sum_{pq \in E(G)} \frac{2\sqrt{d(p)d(q)}}{d(p) + d(q)}. \quad (5)$$

Some more degree-based topological indices are discussed in [14–16]. Aslam et al. computed topological indices of line graphs of subdivision graphs of the i th vertex rooted product graphs [17]. Ahmad et al. computed polynomials of degree-based indices for swapped networks modeled by the optical transpose interconnection [1]. Ahmad computed

degree-based topological indices of the benzene ring in the p -type surface in the 2D network [3].

$$\begin{aligned} M_a(G) &= (8mn + 4m + 4n)2^a + (16mn - 4m - 4n)3^a, \\ R_a(G) &= (4m + 4n)2^{2a} + (16mn - 6m - 6n)3^{2a} + (16mn)6^a. \end{aligned} \quad (6)$$

Vukicević and Furtula computed the topological index based on the ratios of geometrical and arithmetical means of the end vertex degree of edges. In this paper, they introduced a novel topological index based on the end vertex degree and its basic features. They named it as the geometric-arithmetic index [12].

Farahani computed Zagreb indices and Zagreb polynomials of polycyclic aromatic hydrocarbons. In this paper, he computed the first Zagreb index $Z_{g_1}(G)$, second Zagreb index $Z_{g_2}(G)$, and their polynomials $Z_{g_1}(G, x)$ and $Z_{g_2}(G, x)$ of the family of hydrocarbon structure polycyclic aromatic hydrocarbons [5]. Sarkar et al. computed the general Zagreb index of some carbon structures. They computed the general Zagreb index for three carbon allotropes theoretically [15]. Sarkar et al. computed the general Zagreb index of some dendrimer structures. Dendrimers are generally large, complex, and hyperbranched molecules synthesized by repeatable steps with nanometer-scale measurements. They computed the general Zagreb index of some regular dendrimers and hence obtained some vertex degree-based topological indices [16]. Mustapha Chellali computed bounds on the 2-domination number in cactus graphs. He proved that if G is a nontrivial connected cactus graph with $K(G)$ even cycles, then $\gamma_2(G) \geq \gamma_t(G) - K(G)$, and if G is a graph of order n with at most one cycle, then $\gamma_2(G) \geq (n + l - s)/2$ improving Fink and Jacobson's lower bound for trees with $l > s$, where γ_t , l , and s are the total domination number. He also proved that if T is a tree of order $n \geq 3$, then $\gamma_2 \leq \beta(T) + s - 1$ [8].

2. Main Results

We derive the topological indices of the rooted product graph $C_n(P_m)$ of cycle and path graphs. In this work, the mathematical property of the general Zagreb index or (s, t) -Zagreb index of some general ortho- and paracactus chains is studied, and hence, their special cases such as triangular chain cactus T_n , orthochain square cactus O_n , and parachain square cactus Q_n are considered where n denotes the length of the chain, and then we derive some explicit expressions of the same for other degree-based topological indices such as Zagreb indices, forgotten index, redefined Zagreb index, general first Zagreb index, general Randić index, and symmetric division index for particular values of s and t of the general Zagreb index.

3. Topological Indices of the Rooted Product Graph $C_n(P_m)$ of the Cycle and Path Graphs

Let C_n and P_m be the cycle and path graphs on n and m vertices, respectively. Taking n copies of P_m and joining each vertex of C_n with one vertex of P_m , we get the rooted product

FIGURE 1: Example of the rooted product graph $C_n(P_m)$ for $n = 8$ and $m = 5$.

graph $C_n(P_m)$ of the cycle and path graphs. The edge set of $C_n(P_m)$ can be partitioned into the following subsets:

$$\begin{aligned} E_1(C_n(P_m)) &= \{e = pq; d(p) = d(q) = 3\}, \\ E_2(C_n(P_m)) &= \{e = pq; d(p) = 3, d(q) = 2\}, \\ E_3(C_n(P_m)) &= \{e = pq; d(p) = d(q) = 2\}, \\ E_4(C_n(P_m)) &= \{e = pq; d(p) = 2, d(q) = 1\}, \end{aligned} \quad (7)$$

such that $|E_1(C_n(P_m))| = n$, $|E_2(C_n(P_m))| = n$, $|E_3(C_n(P_m))| = n(m-3)$, and $|E_4(C_n(P_m))| = n$. In Figure 1, the rooted product $C_8(P_5)$ is explained.

Theorem 1. If $C_n(P_m)$ is the rooted product graph of cycle and path graphs, then

- (1) $M_1(C_n(P_m)) = M_{1,0}(C_n(P_m)) = 4nm + 2n$
- (2) $M_2(C_n(P_m)) = 1/2 M_{1,1}(C_n(P_m)) = 4nm + 5n$
- (3) $F(C_n(P_m)) = M_{2,0}(C_n(P_m)) = 8nm + 12n$
- (4) $R_e ZM(C_n(P_m)) = M_{2,1}(C_n(P_m)) = 16nm + 42n$
- (5) $M^\alpha(C_n(P_m)) = M_{\alpha-1,0}(C_n(P_m)) = 3^\alpha \times n + 2^\alpha \times n \times (m-2) + 1^\alpha \times n$

$$\begin{aligned} (6) \quad R_\alpha(C_n(P_m)) &= 1/2 M_{\alpha,\alpha}(C_n(P_m)) = n(9)^\alpha + n(6)^\alpha + n(m-3)n(4)^\alpha + n(2)^\alpha \\ (7) \quad SDD(C_n(P_m)) &= M_{1,-1}(C_n(P_m)) = 2n + 13n/6 + n(m-3)(2) + 5/2n \end{aligned}$$

Proof

- (1) We know that the corresponding (s, t) -Zagreb index of the first Zagreb index $M_1(C_n(P_m))$ is $M_{1,0}(C_n(P_m))$.

$$\begin{aligned} M_1(C_n(P_m)) &= M_{1,0}(C_n(P_m)) = ? \\ M_1(C_n(P_m)) &= \sum_{pq \in E(C_n(P_m))} \{d(p) + d(q)\} \\ &= n(3+3) + n(3+2) + n(m-3)(4) + n(3) \\ &= 6n + 5n + 4nm - 12n + 3n \\ M_1(C_n(P_m)) &= 4nm + 2n. \end{aligned} \quad (8)$$

The general Zagreb index of $(C_{\setminus sn}(P_m))$ is given by

$$\begin{aligned} M_{s,t}(C_n(P_m)) &= \sum_{pq \in E(C_n(P_m))} \{d(p)^s d(q)^t + d(p)^t d(q)^s\} \\ &= n(3^s 3^t + 3^t 3^s) + n(3^s 2^t + 3^t 2^s) + n(m-3)(2^s 2^t + 2^t 2^s) + n(2^s 1^t + 2^t 1^s). \\ M_{s,t}(C_n(P_m)) &= n(3^{s+t} + 3^{s+t}) + n(3^s 2^t + 3^t 2^s) \\ &\quad + n(m-3)(2^{s+t} + 2^{s+t}) + n(2^s 1^t + 2^t 1^s). \end{aligned} \quad (9)$$

Putting $s = 1$ and $t = 0$ in equation (1), we have

$$\begin{aligned}
 M_{1,0}(C_n(P_m)) &= n(3+3) + n(3^1 2^0 + 3^0 2^1) \\
 &\quad + n(m-3)(2^1 + 2^1) + n(2^1 1^0 + 2^0 1^1) \\
 &= n(6) + n(3+2) + n(m-3)(4) + n(3) \\
 &= 6n + 5n + 4nm - 12n + 3n \\
 &= 4nm + 2n.
 \end{aligned}
 \tag{10}$$

(2) We know that the corresponding (s, t) -Zagreb index of the second Zagreb index $M_2(C_n(P_m))$ is $1/2 M_{1,1}(C_n(P_m))$.

$$\begin{aligned}
 M_2(C_n(P_m)) &= \frac{1}{2} M_{1,1}(C_n(P_m)) = ? \\
 M_2(C_n(P_m)) &= \sum_{pq \in E(C_n(P_m))} d(p)d(q) \\
 M_2(C_n(P_m)) &= n(9) + n(6) + n(m-3)(4) + n(2) \\
 &= 9n + 6n + 4nm - 12n + 2n \\
 &= 4nm + 5n, \\
 M_{1,1}(C_n(P_m)) &= n(3^1 \times 3^1 + 3^1 \times 3^1) + n(3^1 \times 2^1 + 2^1 \times 3^1) + n(m-3)(2^1 \times 2^1) \\
 &= n(9+9) + n(6+6) + n(m-3)(4+4) + n(2+2) \\
 &= 18n + 12n + n(m-3)(8) + 4n \\
 &= 2[4nm + 5n], \\
 \frac{1}{2} M_{1,1}(C_n(P_m)) &= M_2(C_n(P_m)) = 4nm + 5n.
 \end{aligned}
 \tag{11}$$

(3) We know that the corresponding (s, t) -Zagreb index of the forgotten topological index $F(C_n(P_m))$ is $M_{2,0}(C_n(P_m))$.

Putting $s = 2$ and $t = 0$ in equation (1),

$$\begin{aligned}
 F(C_n(P_m)) &= M_{2,0}(C_n(P_m)) = ? \\
 F(C_n(P_m)) &= \sum_{pq \in E(C_n(P_m))} \{d(p)^2 + d(q)^2\} \\
 &= n(3^2 + 3^2) + n(3^2 + 2^2) \\
 &\quad + n(m-3)(2^2 + 2^2) + n(2^2 + 1^2) \\
 &= 18n + 13n + n(m-3)(8) + 5n \\
 &= 8mn + 12n.
 \end{aligned}
 \tag{12}$$

$$\begin{aligned}
 M_{2,0}(C_n(P_m)) &= n(3^2 \times 3^0 + 3^0 \times 3^2) + n(3^2 \times 2^0 + 3^2 \times 2^0) + n(m-3)(2^2 \times 2^0) \\
 &\quad + 2^0 \times 2^2) + n(2^2 \times 1^0 + 1^2 \times 2^0) \\
 &= n(9+9) + n(9+4) + n(m-3)(4+4) + n(4+1) \\
 &= 18n + 13n + 8mn - 24n + 5n \\
 &= 8mn + 12n, \\
 M_{2,0}(C_n(P_m)) &= F(C_n(P_m)) = 8mn + 12n.
 \end{aligned}
 \tag{13}$$

- (4) We know that the corresponding (s, t) -Zagreb index of the redefined Zagreb index $ReZM(C_n(P_m))$ is $M_{2,1}(C_n(P_m))$.

$$\begin{aligned}
 ReZM(C_n(P_m)) &= M_{2,1}(C_n(P_m)) = ? \\
 ReZM(C_n(P_m)) &= \sum_{pq \in E(C_n(P_m))} d(p)d(q)\{d(p) + d(q)\} \\
 &= n(3)(3)(3+3) + n(3)(2)(3+2) + n(m-3)(2)(2)(2+2) \\
 &\quad + n(2)(1)(2+1) \\
 &= n(9)(6) + n(6)(5) + n(m-3)(4)(4) + n(2)(3) \\
 &= n(54) + n(30) + n(m-3)(16) + n(6) \\
 &= 54n + 30n + 16mn - 48n + 6n. \\
 ReZM(C_n(P_m)) &= 16mn + 42n.
 \end{aligned} \tag{14}$$

Putting $s = 2$ and $t = 1$ in equation (1),

$$\begin{aligned}
 M_{2,1}(C_n(P_m)) &= n(3^2 \times 3^1 + 3^1 \times 3^2) + n(3^2 \times 2^1 + 3^1 \times 2^2) + n(m-3)(2^2 \times 2^1 \\
 &\quad + 2^1 \times 2^2) + n(2^2 \times 1^1 + 1^2 \times 2^1) \\
 &= n(9 \times 3 + 3 \times 9) + n(9 \times 2 + 3 \times 4) + n(m-3)(4 \times 2 + 2 \times 4) \\
 &\quad + n(4 + 2) \\
 &= n(27 + 27) + n(18 + 12) + n(m-3)(8 + 8) + 6n, \\
 &= 54n + 30n + 16mn - 48n + 6n, \\
 M_{2,1}(C_n(P_m)) &= 16mn + 42n. \\
 M_{2,1}(C_n(P_m)) &= ReZM(C_n(P_m)) = 16mn + 42n.
 \end{aligned} \tag{15}$$

- (5) We know that the corresponding (s, t) -Zagreb index of the general Zagreb index $M^\alpha(C_n(P_m))$ is $M_{\alpha-1,0}(C_n(P_m))$.

$$M^\alpha(C_n(P_m)) = M_{\alpha-1,0}(C_n(P_m)) = ?. \tag{16}$$

The general Zagreb index $M^\alpha(C_n(P_m))$ is given by

$$\begin{aligned}
 M^\alpha(C_n(P_m)) &= \sum_{p \in V(C_n(P_m))} d(p)^\alpha. \\
 M^\alpha(C_n(P_m)) &= 3^\alpha \times n + 2^\alpha \times n \times (m-2) + 1^\alpha \times n.
 \end{aligned} \tag{17}$$

Putting $s = \alpha - 1$ and $t = 0$ in equation (1), we get

$$\begin{aligned}
M_{\alpha-1,0}(C_n(P_m)) &= n(3^{\alpha-1} \times 3^0 + 3^0 \times 3^{\alpha-1}) + n(3^{\alpha-1}) \times 2^0 + 3^0 \times 2^{\alpha-1} \\
&\quad + n(m-3)(2^{\alpha-1} \times 2^0 + 2^0 \times 2^{\alpha-1}) + n(2^{\alpha-1} \times 1^0 + 1^{\alpha-1} \times 2^0) \\
&= n(2 \times 3^{\alpha-1}) + n(3^{\alpha-1} + 2^{\alpha-1}) + n(m-3)(2 \times 2^{\alpha-1}) + n(2^{\alpha-1} \\
&\quad + 1^{\alpha-1} \times 2^0) \\
&= 2n \times 3^{\alpha-1} + n3^{\alpha-1} + n \times 2^{\alpha-1} + nm \times 2^\alpha - 3n \times 2^\alpha \\
&\quad + n(2^{\alpha-1} + 1^{\alpha-1} \times 1) \\
&= 3^{\alpha-1}[3n] + 2^{\alpha-1}[2n] + n \times 1^\alpha + mn.2^\alpha - 3n \times 2^\alpha \\
&= 3^\alpha \times n + 2^\alpha \times n + 2^\alpha \times n[m-3] + n \times 1^\alpha \\
&= 3^\alpha \times n + 2^\alpha \times n \times (m-3) + 1^\alpha \times n.
\end{aligned} \tag{18}$$

- (6) We know that the corresponding (s, t) -Zagreb index of the general Randić index $R_\alpha(C_n(P_m))$ is $1/2M_{\alpha,\alpha}(C_n(P_m))$.

$$R_\alpha(C_n(P_m)) = \frac{1}{2}M_{\alpha,\alpha}(C_n(P_m)) = ?. \tag{19}$$

The general Randić index $R_\alpha(G)$ is given by

$$R_\alpha(C_n(P_m)) = \sum_{pq \in E(C_n(P_m))} \{d(p)d(q)\}^\alpha. \tag{20}$$

So,

$$R_\alpha(C_n(P_m)) = n(9)^\alpha + n(6)^\alpha + n(2)^\alpha + n(m-3)(4)^\alpha. \tag{21}$$

Using equation (1),

$$\begin{aligned}
M_{s,t}(C_n(P_m)) &= n(3^{s+t} + 3^{s+t}) + n(3^s 2^t + 3^t 2^s) \\
&\quad + n(m-3)(2^s 2^t + 2^t 2^s) \\
&\quad + n(2^s 1^t + 2^t 1^s).
\end{aligned} \tag{22}$$

Putting $s = \alpha$ and $t = \alpha$ in equation (1), we have

$$\begin{aligned}
M_{\alpha,\alpha}(C_n(P_m)) &= n(3^{2\alpha} + 3^{2\alpha}) + n(3^\alpha \times 2^\alpha + 3^\alpha \times 2^\alpha) + n(m-3)(2^{2\alpha} + 2^{2\alpha}) \\
&\quad + n(2^\alpha \times 1^\alpha + 2^\alpha \times 1^\alpha) \\
&= n(2 \times 3^{2\alpha}) + n(2 \times 2^\alpha 3^\alpha) + n(m-3)(2 \times 2^{2\alpha}) + n(2 \times 2^\alpha) \\
&= 2\{n(9)^\alpha + n(6)^\alpha + n(m-3)n(4)^\alpha + n(2)^\alpha\},
\end{aligned} \tag{23}$$

$$\frac{1}{2}M_{\alpha,\alpha}(C_n(P_m)) = n(9)^\alpha + n(6)^\alpha + n(m-3)n(4)^\alpha + n(2)^\alpha,$$

$$\frac{1}{2}M_{\alpha,\alpha}(C_n(P_m)) = R_\alpha(C_n(P_m)) = n(9)^\alpha + n(6)^\alpha + n(m-3)n(4)^\alpha + n(2)^\alpha.$$

- (7) We know that the corresponding (s, t) -Zagreb index of the symmetric division deg index $SDD(C_n(P_m))$ is $M_{1,-1}(C_n(P_m))$.

$$SDD(C_n(P_m)) = M_{1,-1}(C_n(P_m)) = ?. \tag{24}$$

Putting $s = 1$ and $t = -1$ in equation (1), we have

$$\begin{aligned}
M_{1,-1}(C_n(P_m)) &= n(3^{1-1} + 3^{1-1}) + n(3^1 \times 2^{-1} + 3^{-1} \times 2^1) + n(m-3)(2^{1-1} \\
&\quad + 2^{1-1}) + n(2^1 \times 1^{-1} + 1^1 \times 2^{-1}) \\
&= n(3^0 + 3^0) + n\left(\frac{3}{2} + \frac{2}{3}\right) + n(m-3)(2^0 + 2^0) + n\left(2 + \frac{1}{2}\right) \\
&= n(1+1) + n\left(\frac{9+4}{6}\right) + n(m-3)(1+1) + n\left(\frac{4+1}{2}\right), \\
M_{1,-1}(C_n(P_m)) &= 2n + \frac{13n}{6} + n(m-3)(2) + \frac{5n}{2}, \\
SDD(C_n(P_m)) &= \sum_{pq \in E(C_n(P_m))} \left\{ \frac{d(p)}{d(q)} + \frac{d(q)}{d(p)} \right\} \\
&= n\left(\frac{3}{3} + \frac{3}{3}\right) + n\left(\frac{3}{2} + \frac{2}{3}\right) + n(m-3)(2) + \frac{5n}{2} \\
&= 2n + \frac{13n}{6} + n(m-3)(2) + \frac{5n}{2}, \\
SDD(C_n(P_m)) &= M_{1,-1}(C_n(P_m)) = 2n + \frac{13n}{6} + n(m-3)(2) + \frac{5n}{2}.
\end{aligned} \tag{25}$$

4. Topological Indices of Some General Cactus Chain Graphs

In this section, we find topological indices of two general cactus chain graphs, namely, paracactus chain graph and orthocactus chain graph of cycles. We first consider the paracactus chain graph in which the cut vertices are not adjacent. The paracactus chain graph of cycles is denoted by C_m^n where m is the number of vertices of each cycle and n is the length of the chain. The number of vertices of C_m^n is $mn - n + 1$, and the number of its edges is mn .

Theorem 2. Let C_m^n be the paracactus chain graphs of cycles for $m \geq 3$ and $n \geq 2$; then,

$$M_{(s,t)}(C_m^n) = 4(n-1)2^{s+t}(2^s + 2^t) + (mn - 4n + 4)2^{s+t+1}. \quad \square \tag{26}$$

Proof. The edge set of C_m^n can be partitioned into the following subsets:

$$\begin{aligned}
E_1(C_m^n) &= \{e = pq; d_{C_m^n}(p) = d_{C_m^n}(q) = 2\}, \\
E_2(C_m^n) &= \{e = pq; d_{C_m^n}(p) = 2, d_{C_m^n}(q) = 4\},
\end{aligned} \tag{27}$$

such that $|E_1(C_m^n)| = 2(m-2) + (m-4)(n-2)$ and $|E_2(C_m^n)| = 4(n-1)$.

Then, for the general Zagreb index, we have

$$\begin{aligned}
M_{s,t}(C_m^n) &= \sum_{pq \in E(C_m^n)} \{d(p)^s d(q)^t + d(p)^t d(q)^s\} \\
&= \sum_{pq \in E_1(C_m^n)} (2^s 2^t + 2^t 2^s) + \sum_{pq \in E_2(C_m^n)} (2^s 4^t + 2^t 4^s) \\
&= |E_1(C_m^n)|(2^s 2^t + 2^t 2^s) + |E_2(C_m^n)|(2^s 4^t + 2^t 4^s) \\
&= \{2(m-2) + (m-4)(n-2)\} \times 2^{s+t+1} + 4(n-1) \times 2^{s+t}(2^s + 2^t) \\
&= 4(n-1)2^{s+t}(2^s + 2^t) + (mn - 4n + 4) \times 2^{(s+t+1)}.
\end{aligned} \tag{28}$$

Corollary 1. Let C_m^n be the paracactus chain graph of cycles for $m \geq 3$ and $n \geq 2$; then,

- (1) $M_1(C_m^n) = 4mn + 8n - 8$
- (2) $M_2(C_m^n) = 4mn + 16n - 16$

- (3) $X(C_m^n) = 1/2\{mn - 4n(1 - (\sqrt{2}/3)) + 4(1 - (\sqrt{2}/3))\}$
- (4) $ABC(C_m^n) = 1/\sqrt{2}mn - 2n(\sqrt{2} - \sqrt{3}) + 2(\sqrt{2} - \sqrt{3})$
- (5) $S(C_m^n) = 1/8mn$
- (6) $R_{(-1)}(C_m^n) = 1/2(mn - 2n + 2)$

□

$$(7) R_{-(1/2)}(C_m^n) = (1/2)\{mn - 2n(2 - \sqrt{2}) + 2(2 - \sqrt{2})\}$$

Proof

$$\begin{aligned} M_1(C_m^n) &= \sum_{pq \in E(C_m^n)} \{d(p) + d(q)\} \\ &= 2(m-2) + (m-4)(n-2)(2+2) + 4(n-1)(2+4) \\ &= (2m-4 + mn - 2m - 4n + 8)4 + (4n-4)6 \\ M_1(C_m^n) &= 4nm + 8n - 8. \end{aligned} \quad (29)$$

$$\begin{aligned} M_2(C_m^n) &= \sum_{pq \in E(C_m^n)} d(p)d(q) \\ &= (mn - 4n + 4)4 + (4n - 4)8 \\ &= 4mn - 16n + 16 + 32n - 32M_2(C_m^n) \\ &= 4nm + 16n - 16. \end{aligned} \quad (30)$$

(1) The sum-connectivity index of C_m^n is

$$\begin{aligned} X(C_m^n) &= \sum_{pq \in E(C_m^n)} \frac{1}{\sqrt{d(p) + d(q)}} \\ &= (mn - 4n + 4)\frac{1}{\sqrt{4}} + (4n - 4)\frac{1}{\sqrt{6}} \\ &= \frac{1}{2}(mn - 4n + 4) + \frac{1}{\sqrt{6}}(4n - 4) \\ &= \frac{1}{2}mn - 2n\left(1 - \frac{\sqrt{2}}{\sqrt{3}}\right) + 2\left(1 - \frac{\sqrt{2}}{\sqrt{3}}\right) \\ &\quad \frac{1}{2}\left\{mn - 4n\left(1 - \frac{\sqrt{2}}{\sqrt{3}}\right) + 4\left(1 - \frac{\sqrt{2}}{\sqrt{3}}\right)\right\}. \end{aligned} \quad (31)$$

(2) The atom-bond connectivity index is given by

$$\begin{aligned} ABC(C_m^n) &= \sum_{pq \in E(C_m^n)} \sqrt{\frac{d(p) \times d(q) - 2}{d(p) \times d(q)}} \\ &= (mn - 4n + 4)\sqrt{\frac{2 \times 2 - 2}{2 \times 2}} \\ &\quad + (4n - 4)\sqrt{\frac{2 \times 4 - 2}{2 \times 4}} \\ &= (mn - 4n + 4)\frac{1}{\sqrt{2}} + (4n - 4)\frac{\sqrt{3}}{2} \\ &= \frac{1}{\sqrt{2}}mn - 2n(\sqrt{2} - \sqrt{3}) + (\sqrt{2} - \sqrt{3}). \end{aligned} \quad (32)$$

(3) The Sanskruti index of C_m^n is given by

$$\begin{aligned} S(C_m^n) &= \sum_{pq \in E(C_m^n)} \left\{ \frac{d(p) + d(q) - 2}{d(p) \times d(q)} \right\}^3 \\ &= (mn - 4n + 4)\left(\frac{2+2-2}{2 \times 2}\right)^3 \\ &\quad + (4n - 4)\left(\frac{2+4-2}{2 \times 4}\right)^3 \\ &= \frac{1}{8}\{mn - 4n + 4 + 4n - 4\} \\ &= \frac{mn}{8}. \end{aligned} \quad (33)$$

$$\begin{aligned} R_{-1}(C_m^n) &= \sum_{pq \in E(C_m^n)} \frac{1}{d(p) \times d(q)} \\ &= (mn - 4n + 4)\frac{1}{2 \times 2} + (4n - 4)\frac{1}{2 \times 4} \\ &= \frac{1}{4}(mn - 4n + 4) + \frac{1}{8}(4n - 4) \\ &= \frac{1}{4}(mn - 4n + 4 + 2n - 2) \\ &= \frac{1}{4}(mn - 2n + 2). \end{aligned} \quad (34)$$

$$\begin{aligned} R_{-(1/2)}(C_m^n) &= \sum_{pq \in E(C_m^n)} \frac{1}{\sqrt{d(p) \times d(q)}} \\ &= (mn - 4n + 4)\left(\frac{1}{\sqrt{4}}\right) + (4n - 4)\left(\frac{1}{\sqrt{8}}\right) \\ &= \frac{1}{2}(mn - 4n + 4) + (4n - 4)\frac{1}{2\sqrt{2}} \\ &= \frac{1}{2}\{mn - 2n(2 - \sqrt{2}) + 2(2 - \sqrt{2})\}. \end{aligned} \quad (35)$$

□

If $m = 4$, then we have the graph as shown in Figure 2.

If $m = 6$, then we have the graph as shown in Figure 3.

Putting $m = 4$ and $m = 6$ in equation (1), we get the desired results. Also, putting $m = 4$ and $m = 6$ in Corollary 1, we get results for the above graph.

Now, consider the orthochain cactus graph of cycles where its cut vertices are adjacent. Let this type of cactus chain graph be denoted by CO_m^n where m is the length of each cycle and n is the length of the chain. The number of vertices is $mn - n + 1$, and the number of edges is mn . We calculate the Zagreb index of CO_m^n .

Theorem 3. Let CO_m^n be the orthocactus chain graph of cycles for $m \geq 3$ and $n \geq 2$; then,

FIGURE 2: Example of the paracactus chain graph of cycles for $m = 4$ and $n = n$. FIGURE 3: Example of the paracactus chain graph of cycles for $m = 6$ and $n = n$.

$$M_{s,t}(CO_m^n) = 2(n-2)4^{(s+t)} + 2n \times 2^{(s+t)}(2^s + 2^t) + 2[2(m-2) + (m-3)(n-2)]2^{(s+t)}. \quad (36)$$

$$\begin{aligned} E_1(CO_m^n) &= \{e = pq; d(p) = d(q) = 4\}, \\ E_2(CO_m^n) &= \{e = pq; d(p) = 2, d(q) = 4\}, \\ E_3(CO_m^n) &= \{e = pq; d(p) = d(q) = 2\}, \end{aligned} \quad (37)$$

Proof. The edge set of CO_m^n can be partitioned into the following subsets:

such that $|E_1(CO_m^n)| = (n-1)$, $|E_2(CO_m^n)| = 2n$, and $|E_3(CO_m^n)| = 2(m-2) + (m-3)(n-2)$. The general Zagreb index is

$$\begin{aligned} M_{s,t}(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \{d(p)^s d(q)^t + d(p)^t d(q)^s\} \\ &= \sum_{pq \in E_1(CO_m^n)} (4^s 4^t + 4^t 4^s) + \sum_{pq \in E_2(CO_m^n)} (2^s 4^t + 2^t 4^s) + \sum_{pq \in E_3(CO_m^n)} (2^s 2^t + 2^t 2^s) \\ &= |E_1(CO_m^n)|(4^s 4^t + 4^t 4^s) + |E_2(CO_m^n)|(2^s 4^t + 2^t 4^s) + |E_3(CO_m^n)|(2^s 2^t + 2^t 2^s) \\ &= (n-1)(4^s 4^t + 4^t 4^s) + 2n(2^s 4^t + 2^t 4^s) + 2(m-2) + (m-3)(n-2)(2^s 2^t + 2^t 2^s) \\ &= 2(n-2)4^{s+t} + 2n \times 2^{s+t}(2^s + 2^t) + 2\{(m-2) + (m-3)(n-2)\}2^{s+t} \end{aligned} \quad (38)$$

$$M_{s,t}(CO_m^n) = 2(n-2)4^{s+t} + (mn - 3n + 4)2^{s+t+1} + 2n \times 2s + t + 1(2s + 2t).$$

□

Corollary 2. Let CO_m^n be the orthocactus chain graph of cycles for $m \geq 3$ and $n \geq 2$. Then,

- (1) $M_1(CO_m^n) = 4mn + 8n - 8$
- (2) $M_2(CO_m^n) = 4mn + 20n - 24$
- (3) $GA(CO_m^n) = mn - 2n(1 - (2\sqrt{2}/3))$
- (4) $X(CO_m^n) = 1/2mn + (n/4\sqrt{3})(\sqrt{6} + 4\sqrt{2} - 6\sqrt{3}) + (\sqrt{2} - 1/\sqrt{2})$

$$(5) ABC(CO_m^n) = 1/\sqrt{2}mn + n/4(4\sqrt{3} + \sqrt{14} + 6\sqrt{2}) + (4 - \sqrt{28}/2\sqrt{2})$$

$$(6) S(CO_m^n) = 1/8mn - 37/512n + 37/256$$

$$(7) R_{-1}(CO_m^n) = 1/16(4mn - 7n + 6)$$

$$(8) R_{-2}(CO_m^n) = 1/2mn + 1/4n(2\sqrt{2} - 5) + 1/2$$

Proof

$$\begin{aligned}
M_1(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \{d(p) + d(q)\} \\
&= (n-2)(4+4) + 2n(2+4) + [2(m-2) + (m-3)(n-2)](2+2) \\
&= 8n - 16 + 12n + (2m - 4 + mn - 2m - 3n + 6)4 \\
&= 8n - 16 + 12n + 4mn - 12n + 8 \\
&= 4mn + 8n - 8.
\end{aligned} \tag{39}$$

$$\begin{aligned}
M_2(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \{d(p) \times d(q)\} \\
&= (n-2)(4 \times 4) + 2n(2 \times 4) + (mn - 3n + 2)(2 \times 2) \\
&= 16n - 32 + 16n + 4mn - 12n + 8 \\
&= 4mn + 20n - 24.
\end{aligned} \tag{40}$$

$$\begin{aligned}
GA(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \frac{2\sqrt{d(p) \times d(q)}}{d(p) + d(q)} \\
&= (n-2) \frac{2\sqrt{4 \times 4}}{4+4} + 2n \frac{2\sqrt{2 \times 4}}{2+4} + (mn - 3n + 2) \times 2 \frac{\sqrt{2 \times 2}}{2+2} \\
&= (n-2) \frac{\sqrt{16}}{4} + 2n \frac{2\sqrt{8}}{6} + (mn - 3n + 2) \frac{\sqrt{4}}{2} \\
&= n - 2 + \frac{2}{3}n2\sqrt{2} + mn - 3n + 2 \\
&= mn - 2n \left(1 - \frac{2\sqrt{2}}{3}\right).
\end{aligned} \tag{41}$$

$$\begin{aligned}
X(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \frac{1}{\sqrt{d(p) + d(q)}} \\
&= (n-2) \frac{1}{\sqrt{4+4}} + (2n) \frac{1}{\sqrt{2+4}} + (mn - 3n + 2) \frac{1}{\sqrt{2+2}} \\
&= (n-2) \frac{1}{\sqrt{8}} + (2n) \frac{1}{\sqrt{6}} + (mn - 3n + 2) \frac{1}{\sqrt{4}} \\
&= \frac{1}{2}mn + \frac{n}{2\sqrt{3}}(\sqrt{6} + 4\sqrt{2} - 6\sqrt{3}) + \frac{\sqrt{2} - 1}{\sqrt{2}}.
\end{aligned} \tag{42}$$

$$\begin{aligned}
ABC(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \sqrt{\frac{d(p) \times d(q) - 2}{d(p) \times d(q)}} \\
&= (n-2) \sqrt{\frac{4 \times 4 - 2}{4 \times 4}} + (2n) \sqrt{\frac{2 \times 4 - 2}{2 \times 4}} + (mn - 3n + 2) \sqrt{\frac{2 \times 2 - 2}{2 \times 2}} \\
&= (n-2) \sqrt{\frac{14}{16}} + (2n) \sqrt{\frac{3}{4}} + (mn - 3n + 2) \sqrt{\frac{2}{4}} \\
&= \frac{mn}{\sqrt{2}} - \frac{n}{4} \left(\sqrt{14} + \frac{4}{\sqrt{3}} - \frac{12}{\sqrt{2}} \right) + \left(\frac{4 - \sqrt{28}}{2\sqrt{2}} \right) \\
&= \frac{mn}{\sqrt{2}} - \frac{n}{4} (4\sqrt{3} + \sqrt{14} + 6\sqrt{2}) + \left(\frac{4 - \sqrt{28}}{2\sqrt{2}} \right).
\end{aligned} \tag{43}$$

FIGURE 4: Example of the orthocactus chain graph of cycles for $m = 3$ and $n = n$.

$$\begin{aligned}
 S(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \left(\frac{d(p) + d(q) - 2}{d(p) \times d(q)} \right)^3 \\
 &= (n-2) \left(\frac{4+4-2}{4 \times 4} \right)^3 + 2n \left(\frac{2+4-2}{2 \times 4} \right)^3 + (mn-3n+2) \left(\frac{2+2-2}{2 \times 2} \right)^3 \\
 &= (n-2) \left(\frac{6}{16} \right)^3 + 2n \left(\frac{4}{8} \right)^3 + (mn-3n+2) \left(\frac{2}{4} \right)^3 \\
 &= \frac{1}{8}mn - \frac{37}{512}n + \frac{37}{256}.
 \end{aligned} \tag{44}$$

$$\begin{aligned}
 R_{-1}(CO_m^n) &= \sum_{pq \in E(CO_m^n)} \frac{1}{d(p) \times d(q)} \\
 &= (n-2) \frac{1}{16} + \frac{2n}{8} + (mn-3n+2) \frac{1}{4} \\
 &= \frac{mn}{4} + \frac{n}{16} + \frac{2n}{8} - \frac{3n}{4} + \frac{2}{4} - \frac{2}{16} \\
 &= \frac{1}{16} (4mn - 7n + 6).
 \end{aligned} \tag{45}$$

$$R_{-2}(CO_m^n) = \frac{mn}{2} + \frac{1}{4}n(2\sqrt{2} - 5) + \frac{1}{2}. \tag{46}$$

Corollary 3. Let T_n be the triangular cactus chain for $n \geq 2$; then,

$$M_{s,t}(T_n) = 2^{s+t+2} + n \times 2^{s+t+1} + 2 \times (n-2)4^{s+t}. \tag{47}$$

Proof. Putting $m = 3$ in equation (1), we get the desired result. $\square$

We have an orthocactus graph for $m = 3$ and $n = n$ as shown in Figure 4.

Corollary 4. Let T_n be the triangular cactus chain for $n \geq 2$; then,

- (1) $M_1(T_n) = 20n - 8$
- (2) $M_2(T_n) = 32n - 24$
- (3) $G(T_n) = 3n - 2n(2\sqrt{2}/3)$
- (4) $X(T_n) = 3/2n + n/4\sqrt{3} \quad (\sqrt{6} + 4\sqrt{2} - 6\sqrt{3}) + ((\sqrt{2} - 1)/\sqrt{2})$
- (5) $ABC(T_n) = 3/\sqrt{2}n + n/4 \quad (4/\sqrt{3} + \sqrt{14} + 6\sqrt{2}) + (4 - \sqrt{28}/2\sqrt{2})$
- (6) $S(T_n) = 3/8n - 37/512n + 37/256$
- (7) $R_{-1}(T_n) = 12/16n - 7/16n + 6/16$
- (8) $(R_{-2}) = 3/2n + 1/4n(2\sqrt{2} - 5)$

Proof. Putting $m = 3$ in the results of Corollary 2, we get the desired results. $\square$

5. Conclusion

The topological indices such as the first Zagreb index, second Zagreb index, forgotten index, redefined Zagreb index, and general Randić index have been computed in this paper and have been compared with their corresponding (s, t) -Zagreb indices for the graph $C_n(P_m)$. In this study, some closed expressions of the general Zagreb index of some cactus chain graphs have also been obtained, leading to some other important degree-based topological indices for some particular values of s and t . Results given by these indices can very much be correlated with molecular structures so as to understand their physical and chemical properties. The general Zagreb index of some other graph structures can be computed for further studies.

Data Availability

No data were used to support this study.

Disclosure

This paper has not been published elsewhere, and it will not be submitted anywhere else for publication.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

All the authors contributed equally to this work.

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